STRUCTURAL CHARACTERISATION AND MODELING MECHANICAL PROPERTIES OF PARTICLE REINFORCED METAL-MATRIX COMPOSITES

Theses

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Introduction

There is a long standing scientific interest in predicting effective properties of real heterogeneous materials. Difficulties are mainly related to the lack of adequate three-dimensional characterization techniques of the microstructure, which impede application of existing theoretical approaches. In spite of this scarce understanding of overall properties of real heterogeneous materials the utilization of composites in practice is becoming more and more frequent.

The use of composite materials in practice is mainly determined by their physical properties variable in a wide range and thus can be optimized for special purposes. The different application fields required a large diversity of composite materials, for which reason numerous processing methods were developed. Since their production costs are high, they are mainly used as special parts with extra requirements. Due to their low weight coupled with enhanced mechanical properties primarily, they were used in the space flight technology, military and airplane industry because but with time they come to the front in the rail and automotive industry. As their thermal expansion and heat conduction properties are suitably adjustable they have also become popular in the electronic industry and last but not least in the sports industry due to their especially good elastic properties.

Objectives of the research

There are no satisfying material models for composites in spite of their gradually growing application fields, which could predict their properties accurately. A model cannot be established to describe all details of a composite material, however, the effect of the principal material parameters can be studied, and then estimations can be made about the properties of the modeled composite. These modeling results can be compared to values measured on the real material. One of the aims was that to determine which structural properties are essential, and which play a secondary role in the mechanical behavior of the composites.

In this thesis the modeling possibilities of particle reinforced metal-matrix composites are discussed based on the microstructure map of a real material consisting of AA6061 alloy as matrix and 20% Al_2O_3 ceramic particles as reinforcement obtained by three-dimensional X-ray holotomography. Primarily, the extensively used material testing method, the uniaxial compression was aimed to be simulated, when it is known that the composite is not damaged by small plastic strains (of about 2%).

Thanks to the knowledge of the real microstructure a detailed statistical analysis of the structural properties become possible as well. Although theoretical approximations for estimating elastic properties of heterogeneous materials based on microstructure already exist, there was no comparison between prediction of the theory and measurements on a real material. Because of this I have investigated the applicability of these theoretical approximations to the real material.

Finite element simulations were made for modeling the real materials. The models to be established obtaining accurate results are so large and computationally expensive that it is impossible to model directly an enough large composite volume with fine structural details. Consequently I had to work out adequate modeling strategies that make the accurate estimation of the mechanical properties possible in practice. Furthermore I have tried to optimize modeling of certain mechanical properties so that it assures accurate but relatively short analysis.

Investigation methods and modeling

The AA6061-T6 alloy based Duralcan composite containing 20% Al_2O_3 ceramic particles as reinforcements was used for investigations, which was produced by stir casting then hot extruded. The three-dimensional mapping of the microstructure was performed by X-ray holotomographic reconstruction, which was carried out at beamline ID 19 of the European Synchrotron Radiation Facility in France. A volume with size of 128^3 voxels was cut from the volume with size of 512^3 voxels of a holotomographic reconstruction and used for further structural analysis and modeling (1 voxel = 1.9^3 μm^3).

The stress–strain curve taken by uniaxial compression during mechanical investigations served as the comparison base of the model results. The different models were simulated with the commercial software MSC.Marc/Mentat. The computations were run on a HP J6000 Visual Workstation with two 64-bit PA-RISC processors and 13 GB RAM.

Theses

1. Structural properties [S1]–[S5]

I made a detailed structural analysis based on holotomographic reconstruction. I have determined the characteristic size and shape of the particles by different evaluation point of view. I gave the detailed statistical description about the local environment of particles. I also gave a statistical description valid for the whole composite structure by evaluating the two point probability functions, based on which I could determine the different structural correlation lengths by appropriate criteria. The correlation length obtained from the pair correlation functions was about 4 times larger than the particle size. The knowledge of the correlation lengths is crucial to determine the size of the geometrically representative volume element. Evaluating the coarseness of the structure I described the accuracy of the ergodicity of the real structure. The correlation length originated from the coarseness I found to be about 3 times larger than the particle size in case of the real structure, while in case of the random sphere system only 1.2 times larger than the sphere diameter. Hence I experienced significantly longer structural correlations compared to the case of those models giving the base of the theoretical calculations. During several analyses the structural isotropy in the perpendicular directions to the extrusion axis due to the preparation method of the composite was found which showed up also in the physical properties.

2. Finite element models

I have constructed computerized finite element models based on the results of the purposive structural analysis, which were primarily made in order to get such material models that provide relatively quick results while the unmanageable computational costs are decreased. Analyzing these models the following results were obtained:

2.a Averaging window method [S1]

I modeled the behavior of whole material volume much larger than the representative volume element with the averaging window method based on obscuring the fine details of the local structure. These models were emphasizing mainly the arrangement of particles while their shape was not so accurate. Since this method follows an extrapolation modeling strategy a relatively large modeling error was expected. In spite of this I have obtained quite good approximations of the real data. I ascertained that the spatial arrangement of the particles primarily relates to the work hardening.

2.b Unit cell models [S2]–[S3]

Approaching from the opposite way than in the previous item based on the statistical properties of the local environment of the particles and considering mainly the anisotropy of particle shapes I constructed different one-particle unit cell models. I have concluded about the behavior of the real material on modeling results summed with weights obtained from volumetric distribution functions.

The volume fraction of local models was the main control parameter. I found that the summation by the distribution function which is nearly a Gaussian function gave similar results than the average unit cell model. Based on this model I obtained a good estimation for the plastic stress–strain curve of the real material, however, here should be emphasized its imperfection that it can be applied only with a very limited universality for estimating different mechanical properties, and in addition it does not show the transversal isotropy of the structure. I took also into account the distribution function of the displacements of the particles from the centre position of local volumes and the misalignment of major particle axis with regard to the external load direction. These last two parameters, however, did not significantly improve the final results.

I showed that the volume fraction is the most important material parameter investigating the mechanical properties. Additionally the shape of the particles is also important, but the accurate shape of the particles is not considerable in case of effective material models, only the approximate shape of the contour of particles is essential. Furthermore considering relations between the average aspect ratios of the particles and the surrounding matrix is highly necessary. I ascertained that a more accurate description of the shape of particles improves the initial section near to the ell point of the plastic stress–strain curve.

2.c Multiscale modeling methods [S2]–[S3]

I attempted to approach the mechanical interactions of each local model by multiscale models based on the results of the unit cell models. Simulating multiscale models constructed from randomly arranged basic models, according to statistical distribution functions relating to their volumetric representation, I have found that this approximation did not also provide significantly better results comparing to the average unit cell model. The size of the representative volume element could be estimated according to the model size where the achievement of the random arrangement of the basic models does not count. I estimated that such kind of models is applicable at most up to strain of 2–2.5%, beyond this strain the collective behavior of particles has to be also taken into account.

2.d Direct modeling, mean window method [S4]–[S5]

Investigating the modeling strategies based on the three-dimensional microstructure map directly from the tomographic reconstruction I concluded that similar accuracy can be reached as in case of the former models with these strategies, but significantly better in quality and more universal estimations can be given. The interactions among the particles are considered better, and more general material response can be obtained as well, while the expected transversal symmetry is shown and reasonable estimations can be given for the size of the representative volume element.

Sampling windows cut from the whole reconstructed volume having a volume fraction equal to the mean volume fraction of the composite are called mean windows. Averaging the results of these direct models I estimated the effective properties of the composite. I showed that the mean window method can be applied ubiquitously since the conditions necessary for the use are usually obeyed with good approximations; and it achieves an optimum modeling in the sense that using the least computational resources. It realizes a method which gives generally valid and relatively fast results.

The mean window method excels by the smaller model size and less number of simulated models i.e. lower computational costs required comparing to the direct modeling method based on simple volume covering. This approach gives opportunity to the extensive study of plastic properties.

3. Size of the representative volume element [S4]–[S5]

A relatively large size in case of the direct models based on the volume covering, while a much smaller size in case of the mean window for the representative volume element was obtained. Averaging the response of a few mean windows provides quite good estimations for both the elastic and plastic properties. I found that it is enough to model the mean windows having the size according to the geometrical representative volume element in order to estimate the linear properties, while to investigate the nonlinear material response of the composite about 2 times larger mean windows in linear dimension should be modeled for reaching the modeling accuracy according to the 2% measurement error. This means that in case of elastic properties the size of the volume to be modeled should be at least 3 times larger than the average particle size while in case of plastic properties this factor is about 5–6.

4. Connections between theoretical models and the real structure [S4]–[S5]

During comparison of the results with the theoretical models I ascertained that the isotropic Hashin–Shtrikman two-point bounds, which are narrower than the Voigt's and Reuss' elastic bounds, give reasonable approximations to the elastic constants in case of models with different volume fractions. The Beran–Molyneux–Milton three-point bounds, however, do not give satisfying approximations for the weakly anisotropic structure. However the Willis–Weng anisotropic bounds approximate properly the elastic constants in the different directions in case of the current model structure. I showed that the latter analytical estimation could be effectively used in the practice in case of structures showing statistically transversal isotropy similarly to the investigated composite.

Conclusions

I combined the three-dimensional structural information coming from the holotomographic reconstruction with the finite element method, which was used for estimating the effective mechanical properties of the composite. I pointed out the necessity of the three-dimensional structural analysis, based on which I could well estimate both the elastic and plastic properties by continuum mechanical methods. I determined the size of the representative volume element needed for modeling. In summary, in the knowledge of the reconstructed microstructure, selecting an appropriate modeling strategy, excellent estimations can be provided for the mechanical properties.

I worked out five different modeling strategies, which were evaluated in details. With the help of these models the Young's modulus can be estimated by the practically sufficient accuracy of 2%. I could approximate the plastic stress–strain curve with quite good accuracy until the strain of 1–1.5%, beyond this the models provided larger work hardening than in the measurements. This phenomenon could be the object of a future investigation.

Publications relating to the Ph.D. thesis

[S1] P. Kenesei, A. Borbély, H. Biermann:
Microstructure based three-dimensional finite element model of a particulate reinforced metal-matrix composite
Material Science and Engineering **A387–389** (2004), pp. 852–856.

[S2] P. Kenesei, H. Biermann, A. Borbély:
Structure–property relationship in particle reinforced metal–matrix composites based on holotomography
Scripta Materialia **53** (2005), pp. 787–791.

[S3] P. Kenesei, A. Klohn, H. Biermann, A. Borbély:
Mean field and multiscale modeling of a particle reinforced metal-matrix composite based on microtomographic investigations
Advanced Engineering Materials **8** (2006), pp. 506–510.

[S4] P. Kenesei, H. Biermann, A. Borbély:
Estimation of Elastic Properties of Particle Reinforced Metal-Matrix Composites Based on Tomographic Images
Advanced Engineering Materials **8** (2006), pp. 500–506.

[S5] A. Borbély, P. Kenesei, H. Biermann:
Estimation of effective properties of particle reinforced metal-matrix composites from microtomographic reconstructions
Acta Materialia **54** (2006), pp. 2735–2744.